Integrale Funzionale X Eq di Langevin (a)

caso 1-dim

$$dx = F(x)\,dt + \sqrt{\epsilon}\,dW(t)$$

alla Itô

$$\langle dW(t)\,dW(t')\rangle = \delta(t-t')\,dt$$

e per avere all'equilibrio

$$P(x) = \text{const}\; e^{-\beta V(x)} \qquad \frac{\varepsilon}{2} = k_B T \qquad F(x) = -\frac{dV}{dx}$$

la probabilità condizionata su un passo tempo è

$$P(x_{t+1}\,|\,x_t) = \int d\Delta W_t\, P(\Delta W_t)\, \delta\left(x_{t+1} - x_t - F(x_t)\Delta t - \sqrt{\epsilon}\,\Delta W_t\right)$$

$$P(\Delta W) = \frac{1}{\sqrt{2\pi\Delta t}} \exp\left(-\frac{\Delta W^2}{2\Delta t}\right)$$

$$P(x_{t+1}\,|\,x_t) = \frac{1}{(2\pi\epsilon\Delta t)^{1/2}} \exp\left[-\frac{1}{2\epsilon\Delta t}\left(x_{t+1} - x_t - F(x_t)\Delta t\right)^2\right]$$

$$\frac{1}{2\Delta t}\left(x_{t+1} - x_t - F(x_t)\Delta t\right)^2 = \frac{1}{2}\left(\frac{x_{t+1}-x_t}{\Delta t}\right)^2 \Delta t + \frac{F(x_t)^2}{2}\Delta t - \left(\frac{x_{t+1}-x_t}{\Delta t}\right) F(x_t)\Delta t$$

cfr Risken 4.55

con $D^{(1)} = F \quad D^{(2)} = \varepsilon/2$

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$y \quad x_2 \quad x_1 \quad x$

per 3 slices

$$P(y|x) = \int dx_1 dx_2 \left[\frac{1}{(2\pi\epsilon\Delta t)^{1/2}}\right]^3 \exp\left\{-\frac{1}{\epsilon}\left[\left(\frac{y-x_2}{\Delta t}\right)^2\frac{\Delta t}{2} + \left(\frac{x_2-x_1}{\Delta t}\right)^2\frac{\Delta t}{2} + \left(\frac{x_1-x}{\Delta t}\right)^2\frac{\Delta t}{2} + \right.\right.$$

$$+\frac{F^2(x_1)}{2}\Delta t + \frac{F^2(x_2)}{2}\Delta t + \frac{F^2(x)}{2}\Delta t -$$

$$\left.\left. - \left(\frac{y-x_2}{\Delta t}\right)F(x_2)\Delta t - \left(\frac{x_2-x_1}{\Delta t}\right)F(x_1)\Delta t - \left(\frac{x_1-x}{\Delta t}\right)F(x)\right]\right\}$$

l'ultimo termine nell'esponente fa

$$-\left[yF(x_2) + x_2\big(F(x_1)-F(x_2)\big) + x_1\big(F(x)-F(x_1)\big) - xF(x)\right]$$

$$F(x_t) = -\frac{V(x_t)-V(x_{t-1})}{x_t - x_{t-1}} \quad \underline{\text{oppure}} \quad \frac{V(x_{t+1})-V(x_t)}{x_{t+1}-x_t} \quad ?$$

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se prendiamo la seconda l'ultimo termine è

$$-\left[(V(y)-V(x_2)) + (V(x_2)-V(x_1)) + (V(x_1)-V(x))\right] =$$

$$= -(V(y)-V(x))$$

$$\boxed{P(y|x) = \frac{e^{-\frac{V(x)-V(y)}{\epsilon}}}{(2\pi\epsilon\Delta t)^{1/2}} \int \prod_1^L{}_k dx_k \, e^{-S/\epsilon}}$$

$$\boxed{S = \frac{1}{2}\left(\sum_0^L{}_k \left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 \Delta t + F^2(x_k)\Delta t\right) \qquad \begin{array}{l} x_{L+1} = y \\ x_0 = x \end{array}}$$

(L+1 slices)

cfr Risken $\underline{4.59}$

posso dividere l'integrale fra $[0,\beta]$ in L slices ⓓ

la parte diagonale della matrice densità

$$P_{Quant}(x) = \langle x | e^{-\beta H} | x \rangle$$

risulta analoga alla probabilità condizionata

$$\boxed{P_{Langevin}(x\beta | x 0) \quad \text{se}}$$

$$\boxed{\epsilon = \frac{\hbar^2}{m} \qquad F^2_{Langevin}(x) = 2\frac{\hbar^2}{m} V(x)}$$

schrödinger

o analogamente divido $[0, \beta\hbar]$ in L slices ed allora

$$\boxed{P_{Langevin}(x \beta\hbar | x\, 0) \quad \text{se}}$$

$$\boxed{\epsilon = \frac{\hbar}{m} \quad \text{ed} \quad F^2(x) = 2\frac{V(x)}{m}}$$

Diffusione t. imm

$$\langle |X(\tau) - X(0)|^2 \rangle$$

$$X^2(\tau) + X^2(0) - X(\tau)\, X - X\, X(\tau)$$

$$e^{-\beta H} e^{-\tau H} x^2 e^{\tau H} + \langle x^2 \rangle - e^{-\beta H} e^{-\tau H} x\, e^{\tau H} x - e^{-\beta H} x\, e^{-\tau H} x\, e^{\tau H}$$

$$e^{-(\beta-\tau) H} x^2 e^{+\tau H} + x^2 + e^{-(\beta-\tau) H} x\, e^{\tau H} x$$

$$e^{-\beta H} x\, e^{-\tau H} x$$

$$e^{-(\beta-\tau) H} x^2 e^{-\tau H} + \rho_\beta x^2 - 2\, e^{-(\beta-\tau) H} x\, e^{-\tau H} x$$

$$\rho_{\beta-\tau} x^2 \rho_\tau + \rho_\beta x^2 - 2 \rho_{\beta-\tau} x\, \rho_\tau x$$

$$|\rho_{\beta-\tau} x\, \rho_\tau - x|^2 \qquad e^{-(\beta-\tau)}$$

$$\rho_{\beta-\tau} (x-y)^2 \rho_\tau$$

$$\rho_{\beta-\tau} (x$$

$$\rho_{\beta-\tau}(y,x)\,(x^2 + y^2 - 2xy)\,\rho_\tau(x,y)$$

$$\rho_{\beta-\tau} x^2 \rho_\tau + x^2 - 2 \rho_{\beta-\tau} x\, \rho_\tau x$$

$$\int dx\, dy \quad \rho_{\beta-\tau}(x,y)\, y^2 \rho_\tau(y,x) + \rho_\beta(x,y)\, y^2 \cancel{\delta(x-y)} - 2 \rho_{\beta-\tau}(x,y)\, y\, \rho_\tau(y,x)\, x$$

Sistema a 2 livelli

$$\langle 1|X|1\rangle = 0$$

$$\langle 2|X|2\rangle = 0$$

$$\langle 1|X|2\rangle\langle 2|X|1\rangle e^{-(\beta-\tau)[E_1-\cancel{E_2}]} e^{\tau E_2} +$$

$$+ \langle 2|X|1\rangle\langle 1|X|2\rangle e^{-(\beta-\tau)E_2} e^{\tau E_1}$$

$$\langle 1|X|2\rangle = X$$

$$\langle |X(\tau)-X(0)|^2\rangle = 2\langle X^2\rangle - 2\frac{1}{Z}\Big(e^{-\beta E_1} X^2 e^{\tau E_2} e^{\tau E_1} +$$

$$+ e^{-\beta E_2} X^2 e^{\tau E_1} e^{\tau E_2}\Big)$$

$$= 2\langle X^2\rangle - 2X^2 e^{\tau(E_1+E_2)}$$

Numeri di occupazione

$|0,0\rangle$ ← ~~$\psi_0(x_1)\psi_0(x_2)$~~ non ho particelle

$|1,0\rangle$ 1 particella in E_1 $\psi_1(x_1)$

$|0,1\rangle$ 1 particella in E_2 $\psi_2(x_1)$

$|2,0\rangle$ 2 particelle in E_1 → $\psi_1(x_1)\psi_1(x_2)$

$|1,1\rangle$ 1 part in E_1 1 in E_2 $\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) \pm \psi_2(x_1)\psi_1(x_2)\right)$

le energie

$$H = \Sigma_K n_K E_K = \sum_i^N H_i$$

particelle indipendenti

n_K: numero di particelle stato k

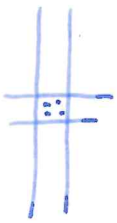
E_K: energia di singola particella

se particelle identiche H_i indip i!

$$H = \qquad H^{(1)}|k\rangle = E_k|k\rangle$$

E_k: singola particella

anche classicamente ho una energia di sistemi indipendenti



$$E = \sum_i^{M} n_i \varepsilon_i$$

n_i: # di particelle presenti nella i-esima celletta del μ-spazio

μ-spazio diviso in M celle di volume h^3